201-14929A

HIGH PRODUCTION VOLUME (HPV)

CHALLENGE PROGRAM

TEST PLAN

For

Alkenes, C15-C18 alpha, reaction products with sulfurized dodecyl phenol, calcium salt, sulfurized (CAS No. 72275-86-6)

Prepared by
The American Chemistry Council
Petroleum Additives Panel
Health, Environmental, and Regulatory Task Group

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LIST OF MEMBER COMPANIES IN THE
HEALTH, ENVIRONMENTAL AND REGULATORY TASK GROUP

The Health, Environmental, and Regulatory Task Group (HERTG) of the American Chemistry Council Petroleum Additives Panel includes the following member companies:

Chevron Oronite Company, LLC

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1.0 INTRODUCTION

In March 1999, the American Chemistry Council (formerly the Chemical Manufacturers Association) Petroleum Additives Panel Health, Environmental, and Regulatory Task Group (HERTG), and its participating member companies committed to address for certain chemicals listed under the Environmental Protection Agency (EPA) High Production Volume (HPV) Chemical Challenge Program. This test plan follows up on that commitment.

Specifically, this test plan sets forth how the HERTG intends to address testing information for the following substance:

- Alkenes, C15-C18 alpha, reaction products with sulfurized dodecyl phenol, calcium salt, sulfurized (CAS No. 72275-86-6)

This document indicates the findings of the data review process, and sets forth a proposed test plan.

In preparing this test plan the following steps were undertaken:

Step 1: A review of the literature and confidential company data was conducted on the physicochemcial properties, mammalian toxicity endpoints, and environmental fate and effects for Alkenes, C15-C18 alpha, reaction products with sulfurized dodecyl phenol, calcium salt, sulfurized (CAS No. 72275-86-6) using its CAS number, CAS name, and synonyms. Searches included the following sources: MEDLINE, BIOSIS, CANCERLIT, CAPLUS, CHEMLIST, EMBASE, HSDB, RTECS, EMIC, and TOXLINE databases; the TSCATS database for relevant unpublished studies on these chemicals; and standard handbooks and databases (e.g., Sax, CRC Handbook on Chemicals, IUCLID, Merck Index, and other references) for physicochemical properties.

Step 2: The compiled data was evaluated for adequacy in accordance with the EPA guidance documentation.

2.0 GENERAL SUBSTANCE INFORMATION

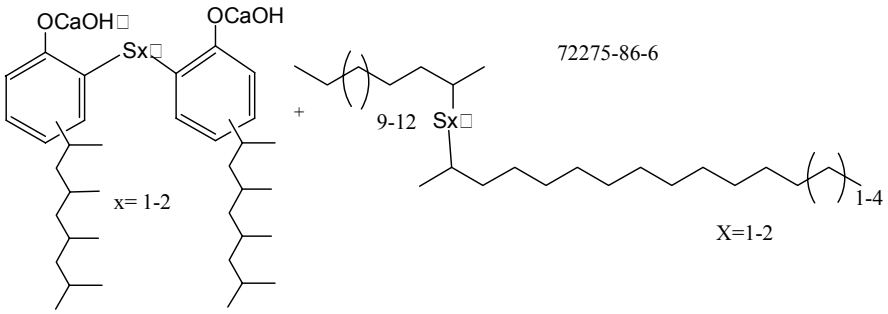
The substance that is the subject of this test plan is used as a petroleum additive in petroleum base stocks. The chemical name, CAS Registry Number, molecular weight and chemical structure for this substance are presented below.

Chemical Name: Alkenes, C15-C18 alpha, reaction products with sulfurized dodecyl phenol, calcium salt, sulfurized

Chemical Abstract Service Registry Number: 72275-86-6

Molecular Weight Range: 454.88-699.13 gm/mol

Chemical Structure:



3.0 EXPOSURE INFORMATION

Manufacture

This material is prepared by sulfurizing tetrapropenyl phenol with excess elemental sulfur and neutralizing the sulfurized alkyl phenol with calcium hydroxide. In a second step in the same reactor after the reaction is cooled, a mixture of C15-C18 alpha-olefins is added. The olefins react with the remaining un-reacted sulfur producing a sulfurized olefin. The solvent in which these reactions occur is highly refined lubricating base oil, and the concentration of highly refined lubricant base oil in the commercial component is 19 wt.%.

This material is a physical mixture of CAS No. 67762-55-4, an alkyl sulfide that is a member of the Alkyl Sulfide category submission by the HERTG to the EPA HPV Chemical Challenge on March 28, 2000, and CAS No. 122384-85-4, an alkyl phenate sulfide that is a member of the Alkyl Phenate Sulfide category in preparation for submission by the HERTG to the ICCA HPV Chemical Challenge. Even though this material is made in one reaction, it remains a physical mixture of sulfurized calcium phenate and sulfurized alkyl sulfides. Both materials can be separated from the substance using HPLC indicating that there is no reaction between a sulfurized alkyl phenol and the additional olefin added in step two. This point justifies the use of data for the alkyl sulfide defined by CAS No. 67762-55-4 (or in some instances, data from a similar lower molecular weight alkyl sulfides defined by CAS No. 68511-50-2 and CAS No. 67124-09-8) and the alkyl phenate sulfide defined by CAS No. 122384-85-4 to augment the test data for CAS No. 72275-86-6 and supply data when data for CAS No. 72275-86-6 could not otherwise be located.

Use

This substance is used as a detergent and inhibitor in crankcase lubricants. It provides detergency to prevent deposit formation on engine parts such as on pistons and as an inhibitor to prevent bulk oil oxidation. The concentration of this substance ranges from 2.0 wt-% to 18.0 wt-% in additive packages. When these additive packages are blended into finished lubricants, the final concentration of this substance ranges from 0.5 wt-% to 3.0 wt-%.

4.0 PHYSICOCHEMICAL PROPERTIES

4.1 Summary of Available Data

The chemical structures for Alkenes, C15-C18 alpha, reaction products with sulfurized dodecyl phenol, calcium salt, sulfurized are shown in Table 2. These structures are essentially identical to an alkyl sulfide, Alkenes, C15-C18 alpha-, sulfurized (CAS No. 67762-55-4), and an alkyl phenate sulfide, Phenol, tetrapropenyl-, sulfurized, calcium salts (CAS No. 122384-85-4), and are similar to 1-Propene, 2-methyl-, sulfurized (CAS No. 68511-50-2), which is also an alkyl sulfide. The chemical structures of these substances are also shown in Table 2.

Alkenes, C15-C18 alpha, reaction products with sulfurized dodecyl phenol, calcium salt, sulfurized are a liquid at ambient temperatures. The viscosity of this substance is 94 cSt at 100^{o}C, and the specific gravity is 1.00 at 15.6 ^{o}C.

No published or unpublished data were located for the melting point, boiling point, vapor pressure, water solubility or octanol/water partition coefficient for Alkenes, C15-C18 alpha, reaction products with sulfurized dodecyl phenol, calcium salt, sulfurized. Data located for Phenol, tetrapropenyl-, sulfurized, calcium salts (CAS No. 122384-85-4) are also presented in Table 3.

4.2 Data Assessment and Test Plan for Physicochemical Properties

No adequate and reliable data were located for the boiling point and vapor pressure for alkenes, C15-C18 alpha, reaction products with sulfurized dodecyl phenol, calcium salt, sulfurized. However, Alkenes, C15-18 alpha, reaction product with sulfurized dodecyl phenol, calcium salt, sulfurized is liquid at ambient temperatures (thus melting point is not applicable). The octanol/water partition coefficient and water solubility of alkenes, C15-18 alpha, reaction product with sulfurized dodecyl phenol, calcium salt, sulfurized are indicative of the two structurally similar components (CAS Nos. 67762-55-4 and 122384-85-4). Therefore, testing is not proposed for water solubility or octanol/water partition coefficient. The other physicochemical properties will be measured as indicated in Table 1.

5.0 ENVIRONMENTAL FATE DATA

The environmental fate of a substance and its degradation by-products, including their partitioning among environmental compartments, are dependent on the physicochemical properties. The important environmental degradation pathways for lubricant additives are biodegradation, hydrolysis, and photodegradation.

5.1 Biodegradability

5.1.1 Summary of Available Data

Biodegradation, the measurement of the potential of a compound to be degraded by microorganisms, has been not been evaluated for Alkenes, C15-C18 alpha, reaction

products with sulfurized dodecyl phenol, calcium salt, sulfurized based on our inability to locate any studies in the published or unpublished scientific literature.

Biodegradation data exist for Phenol, tetrapropenyl-, sulfurized, calcium salts (CAS No. 122384-85-4). Although data could not be located for Alkenes, C15-C18 alpha-, sulfurized (CAS No. 67762-55-4), data are available for a structurally similar lower molecular weight alkyl sulfide, 1-Propene, 2-methyl-, sulfurized (CAS No. 68511-50-2). Data for both of these substances indicates that they are not readily biodegradable.

5.1.2. Data Assessment and Test Plan for Biodegradability

Based on the similarities in chemical structures and physicochemical properties for all of these substances, it is scientifically justifiable to extrapolate the data from the similar Alkyl sulfide and Alkyl phenate sulfide to Alkenes, C15-C18 alpha, reaction products with sulfurized dodecyl phenol, calcium salt, sulfurized (CAS No. 72275-86-6) and conclude that this substance also is not readily biodegradable. Therefore, additional biodegradation testing is not proposed.

5.2 Hydrolysis

5.2.1 Summary of Available Data

No published or unpublished hydrolysis data for members of the Alkenes, C15-18 alpha, reaction products with sulfurized dodecyl phenol, calcium salt, sulfurized were located.

5.2.2 Data Assessment and Test Plan for Hydrolysis

Hydrolysis, the reaction in which a water molecule or hydroxide ion substitutes for another atom or group of atoms present in an organic molecule, has not been evaluated for Alkenes, C15-18 alpha, reaction products with sulfurized dodecyl phenol, calcium salts, sulfurized. However, an examination of the chemical structure suggests that Alkenes, C15-18 alpha, reaction products with sulfurized dodecyl phenol, calcium salt, sulfurized, do not contain functional groups that are susceptible to hydrolytic degradative mechanisms.[1] Therefore, this fate process will not contribute to the degradative loss of chemical components in this category from the environment. Since Alkenes, C15-18 alpha, reaction products with sulfurized dodecyl phenol, calcium salt, sulfurized, do not contain functional groups that are susceptible to hydrolytic degradative mechanisms, testing these substances for hydrolysis is not needed to adequately evaluate this endpoint. Therefore, no hydrolysis testing is proposed for this category**.**

5.3 Photodegradation

5.3.1 Summary of Available Data

[1] Lyman, W. J., W. F. Reehl, and D. H. Rosenblatt. 1982. Handbook of Chemical Property Estimation Methods. McGraw-Hill Book Co., New York, NY, USA.

No published or unpublished photodegradation studies for Alkenes, C15-C18 alpha, reaction products with sulfurized dodecyl phenol, calcium salt, sulfurized were located.

5.3.2 Data Assessment and Test Plan for Photodegradation

The Atmospheric Oxidation Potential (AOP) will be characterized for each of the separate components (CAS Nos. 67762-55-4 and 122384-85-4) of Alkenes, C15-18 alpha, reaction products with sulfurized dodecyl phenol, calcium salt, sulfurized using the modeling program AOPWIN. This computer simulation is recommended in the Agency's recently released structure activity review (SAR) guidance for HPV chemicals.

5.4 Fugacity Modeling

5.4.1 Summary of Available Data

No published or unpublished fugacity-based multimedia fate modeling studies were located for Alkenes, C15-C18 alpha, reaction products with sulfurized dodecyl phenol, calcium salt, sulfurized.

5.4.2 Test Plan for Fugacity

The relative distribution of Alkenes, C15-C18 alpha, reaction products with sulfurized dodecyl phenol, calcium salt, sulfurized among environmental compartments will be evaluated using Level I Fugacity modeling. EPA states in the document, "Determining the Adequacy of Existing Data", that Level I fugacity modeling is acceptable to estimate transport/distribution values. The Level I model utilizes input of basic chemical properties, including molecular weight, vapor pressure, and water solubility to calculate percent distribution within a standardized environment.

Input data to run the Level I model will require an additional computer model to estimate physical/chemical properties from a structure if measured values are not available. The model used for this purpose will be EPIWIN, version 3.02[2], which was developed by the Syracuse Research Corporation. EPIWIN includes algorithms for estimating all physical and chemical properties needed for the Level 1 model.

6.0 ECOTOXICOLOGY DATA

6.1 Aquatic Toxicity

6.1.1 Summary of Available Data

- OECD Guideline 203 (*Fish, Acute Toxicity Test*): The 96-hour LL_{50} of Alkenes, C15-C18 alpha, reaction products with sulfurized dodecyl phenol, calcium salt, sulfurized determined in sheepshead minnow is > 10,000 mg/L WAF. The 96-hour NOEL is 1000 mg/L WAF.

[2] Environmental Science Center- Syracuse Research Corporation- EPI for windows.

- The 96-hour EL_{50} of Alkenes, C15-C18 alpha, reaction products with sulfurized dodecyl phenol, calcium salt, sulfurized determined in brown shrimp is 2600 mg/L WAF. The 96-hour NOEL is 100 mg/L WAF.

- Studies in daphnia (OECD Guideline 202, *Daphnia sp., Acute Immobilization Test and Reproduction Test*) or algae (OECD Guideline 201, *Alga, Growth Inhibition Test*) were not located in the published or unpublished scientific literature.

  Acute aquatic toxicity data in three species exist for Phenol, tetrapropenyl-, sulfurized, calcium salts (CAS No. 122384-85-4). Although data could not be located for Alkenes, C15-C18 alpha-, sulfurized (CAS No. 67762-55-4), data in three species exist for a structurally similar lower molecular weight alkyl sulfide, 1-Propene, 2-methyl-, sulfurized (CAS No. 68511-50-2). The data generally indicates that these two substances are of low concern for acute aquatic toxicity.

6.2.1 Data Assessment and Test Plan for Acute Aquatic Toxicity

The available acute aquatic toxicity data in fish and brown shrimp are adequate and reliable and are consistent with the data for the similar Alkyl sulfide and Alkyl phenate sulfide. Based on the similarities in chemical structure and physicochemical properties for all of these substances, it is scientifically justifiable to extrapolate the data for daphnia and algae from the similar Alkyl sulfide and Alkyl phenate sulfide to Alkenes, C15-C18 alpha, reaction products with sulfurized dodecyl phenol, calcium salt, sulfurized (CAS No. 72275-86-6) and conclude that this substance is a low concern for acute aquatic toxicity as well. Therefore, additional acute aquatic toxicity testing is not proposed.

7.0 MAMMALIAN TOXICOLOGY DATA

7.1 Acute Mammalian Toxicity

7.1.1 Summary of Available Data

The acute toxicity of Alkenes, C15-C18 alpha, reaction products with sulfurized dodecyl phenol, calcium salt, sulfurized has been evaluated via the oral and dermal route:

- OECD Guideline 401 *Acute Oral Toxicity* (similar to method FHSA 16 CFR1500.3): The acute oral LD_{50} in the rat is > 5.0 g/kg indicating a low concern for acute toxicity.

- OECD Guideline 402 (*Acute Dermal Toxicity*): The acute dermal LD_{50} in the rabbit is > 5.0 indicating a low concern for acute toxicity.

Acute toxicity data exists for the similar Alkyl sulfides and Alkyl phenate sulfide and are presented in Table 6. The results of these tests also indicate a low concern for acute toxicity.

7.1.2 Data Assessment and Test Plan for Acute Mammalian Toxicity

Adequate and reliable acute oral and dermal toxicity tests were performed for Alkenes, C15-C18 alpha, reaction products with sulfurized dodecyl phenol, calcium salt, sulfurized. Additional acute mammalian toxicity testing is not proposed.

7.2. Mutagenicity

7.2.1 Summary of Available Data

The genetic toxicity of Alkenes, C15-C18 alpha, reaction products with sulfurized dodecyl phenol, calcium salt, sulfurized has been evaluated for point mutations in test systems that evaluate base-pair substitution and frame shift mutations (Table 7):

- OECD Guideline 471 (*Bacterial Reverse Mutation Test*): A *Salmonella typhimurium* point mutation assay exists for Alkenes, C15-C18 alpha, reaction products with sulfurized dodecyl phenol, calcium salt, sulfurized. The data indicate that this substance is not mutagenic in this test system.

Studies of Alkenes, C15-C18 alpha, reaction products with sulfurized dodecyl phenol, calcium salt, sulfurized in test systems for chromosomal aberrations were not located.

Genetic toxicity studies for point mutations and chromosome aberrations exist for Phenol, tetrapropenyl-, sulfurized, calcium salts (CAS No. 122384-85-4). The data indicate that this substance is neither mutagenic nor clastogenic in these test systems.

Point mutation studies exist for structurally similar lower molecular weight alkyl sulfides, Alkenes, C15-C18 alpha-, sulfurized (CAS No. 67762-55-4) and 1-Propene, 2-methyl-, sulfurized (CAS No. 68511-50-2), and the data indicate that these substances are not mutagenic in this test system. In addition, a genetic toxicity study for chromosome aberrations exists for a C12-C16 analog of Alkenes, C15-C18 alpha-, sulfurized (CAS No. 67762-55-4), and the data indicate that this substance is not clastogenic in this test system.

7.2.2 Data Assessment and Test Plan for Mutagenicity Toxicity

An adequate and reliable *Salmonella typhimurium* point mutation assay is available for Alkenes, C15-C18 alpha-, reaction products with sulfurized dodecyl phenol, calcium salt, sulfurized. Additional adequate and reliable point mutation studies are negative for the similar Alkyl sulfide and Alkyl phenate sulfide. Based on the similarities in chemical structure and physicochemical properties for all of these substances, it is scientifically justifiable to extrapolate the data for chromosome aberrations from the similar Alkyl sulfides and Alkyl phenate sulfide to Alkenes, C15-C18 alpha, reaction products with sulfurized dodecyl phenol, calcium salt, sulfurized (CAS No. 72275-86-

6) and conclude that this substance is a low concern for genetic toxicity as well. Therefore, additional genetic toxicity testing is not proposed.

7.3 Repeated-dose, Reproductive and Developmental Toxicity

7.3.1 Summary of Repeated-Dose Toxicity Data

The repeated dose toxicity of Alkenes, C15-C18 alpha, reaction products with sulfurized dodecyl phenol, calcium salt, sulfurized has been evaluated in a 28-day repeated-dose dermal toxicity study in rats (Table 8):

- OECD Guideline 410 (*Repeated Dose Dermal Toxicity: 21/28-day Study*): Minimal signs of systemic toxicity were observed in this study. The NOAEL is 100 mg/kg/day.

A repeated-dose toxicity study also exists for Phenol, tetrapropenyl-, sulfurized, calcium salts (CAS No. 122384-85-4). Although data could not be located for Alkenes, C15-C18 alpha-, sulfurized (CAS No. 67762-55-4), data exist for a structurally similar lower molecular weight alkyl sulfide, 2-propanol, 1-(tert-dodecylthio)- (CAS No. 67124-09-8). All reviewed studies indicate that these substances are also a low concern for repeated dose toxicity.

No published or unpublished reproductive or developmental toxicity tests for Alkenes, C15-C18 alpha, reaction products with sulfurized dodecyl phenol, calcium salt, sulfurized were located (Table 8). However, a reproductive toxicity screening toxicity test exists for phenol, tetrapropenyl-, sulfurized, calcium salts (CAS No. 122384-85-4). Although data could not be located for Alkenes, C15-C18 alpha-, sulfurized (CAS No. 67762-55-4), data exist for a structurally similar lower molecular weight alkyl sulfide, 2-propanol, 1-(tert-dodecylthio)- (CAS No. 67124-09-8). Both reproductive toxicity studies did not show any adverse effects on fertility or any other reproductive endpoints.

7.3.2 Data Assessment and Test Plan for Repeated-dose Toxicity

An adequate and reliable repeated-dose toxicity study exists for alkenes, C15-C18 alpha, reaction products with sulfurized dodecyl phenol, calcium salt, sulfurized. Although a reproductive toxicity study for this substance could not be located, adequate and reliable reproductive toxicity studies are negative for the similar Alkyl sulfide and Alkyl phenate sulfide. Thus, based on the similarities in chemical structure and physicochemical properties for all of these substances, it is scientifically justifiable to extrapolate the data for reproductive toxicity from the similar Alkyl sulfides and Alkyl phenate sulfide to Alkenes, C15-C18 alpha, reaction products with sulfurized dodecyl phenol, calcium salt, sulfurized (CAS No. 72275-86-6) and conclude that this substance is also a low concern for reproductive toxicity. Therefore, additional reproductive and developmental toxicity testing is not proposed.

SUMMARY

The following tables summarize the available data and proposed testing on alkenes, C15-C18 alpha, reaction products with sulfurized dodecyl phenol, calcium salt, sulfurized.

Table 1
Summary Table of Available Data and Proposed Testing on
Alkenes, C15-C18 alpha, reaction products with sulfurized dodecyl phenol, calcium salt, sulfurized (CAS No. 72275-86-6)

CAS No.: 7225-86-6	Study Results	Testing Proposed
Physical/Chemical Characteristics		
Melting Point	Liquid at ambient temperatures	No
Boiling Point	No Data Located	Yes
Vapor Pressure	No Data Located	Yes
Water Solubility	Indicative of two structurally similar components	No
Partition Coefficient	Indicative of two structurally similar components	No
Environmental Fate		
Biodegradation	Not readily biodegradable	No
Hydrolysis	Not susceptible to hydrolytic degradative mechanisms	No
Photodegradation	No Data Located	Model with AOPWIN
Fugacity	No Data Located	Model with EPIWIN
Ecotoxicity		
Acute Toxicity to Fish	96 hr LC50: >10,000 mg/L WSF	No
Acute Toxicity to Invertebrates	96 hr EL50 is 2600 mg/L WAF (brown shrimp) 96 hr NOEL is 100 mg/L WAF (brown shrimp)	No
Acute Toxicity to Algae	No Data Located Bridging from similar substances	No
Mammalian Toxicity		
Acute Toxicity	Oral LD50 > 5 g/kg (rat) Dermal LD50 > 5 g/kg (rabbit)	No
Repeated Dose Toxicity	30 wt% (300 mg/kg/day) in mineral oil Changes in serum chemistry parameters 10 wt% (100 mg/kg/day) in mineral oil No signs of systemic toxicity 3 wt% (30 mg/kg/day) in mineral oil No signs of systemic toxicity	No
Reproductive Toxicity *Developmental Toxicity*	No Data Located Bridging from similar substances	No
Genotoxicity		
Gene Mutation	Not mutagenic	No
Chromosomal Aberration	No Data Located Bridging from similar substances	No

Table 2. Chemical Structures of Alkenes, C15-C18 alpha, reaction products with sulfurized dodecyl phenol, calcium salt, sulfurized (CAS No. 72275-86-6)

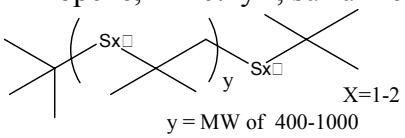
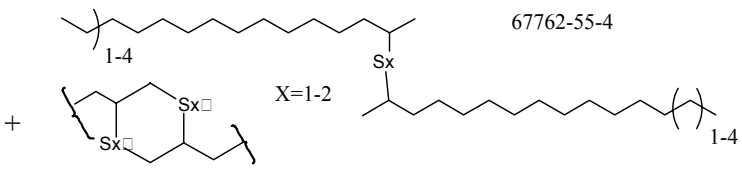
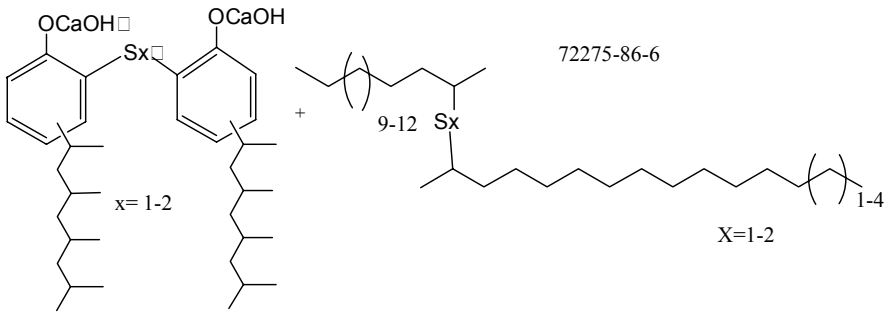
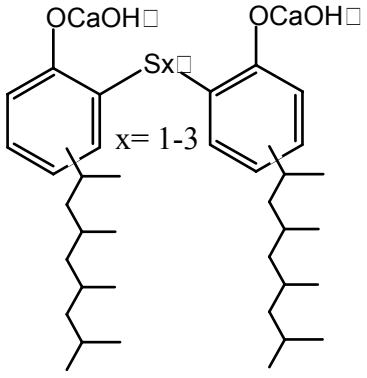
CAS Number	Chemical Structure
68511-50-2 Alkyl Sulfide	1-Propene, 2-methyl-, sulfurized  68511-50-2 y = MW of 400-1000
67762-55-4 Alkyl Sulfide	Alkenes, C15-C18 alpha-, sulfurized 
72275-86-6 Reaction Mixture of Alkyl Sulfide and Alkyl Phenate Sulfides	
122384-85-4 Alkyl Phenate Sulfide	

Table 3. Physicochemical Properties of Alkenes, C15-C18 alpha, reaction products with sulfurized dodecyl phenol, calcium salt, sulfurized (CAS No. 72275-86-6)

CAS Number	Melting Point (°C)	Boiling Point (°C)	Vapor Pressure (Pa @ 25°C)	Water Solubility (mg/L)	Log Kow[5]
68511-50-2 Alkyl Sulfide	147.5-329.3[1]	409.4-749.8[1]	3.63×10^{-16}-3.71×10^{-5} [1]	3.29×10^{-18}-3.94×10^{-4}	7.99-15.23[1]
67762-55-4 Alkyl Sulfide	186.9-213.8[1]	504.5-537.8[1]	$0.39\text{-}5.69 \times 10^{-8}$ [1]	$0.164\text{-}1.59 \times 10^{-10}$ [1]	16.00-16.95[1]
72275-86-6	Liquid at ambient temperatures	Test	Test	No testing proposed Bridging	No Testing proposed Bridging
122384-85-4 Alkyl Phenate Sulfide	257[1]	596[1]	$< 1.7 \times 10^{-4}$ [2]	0.082[3]	> 6.6[3]

[1] Modeling data, EPIWIN
[2] Based on partial pressure of the highly refined lubricant base oil [CONCAWE (1997) Lubricating Oil Basestocks. Product Dossier No. 97/108].
[3] Based on data for an overbased alkyl phenate sulfide (122384-87-6)

Table 4. Evaluation of Environmental Fate Information for Alkenes, C15-C18 alpha, reaction products with sulfurized dodecyl phenol, calcium salt, sulfurized (CAS No. 72275-86-6)

CAS Number	BIODEGRADABILITY Available Data & Proposed Testing	HYDROLYSIS Available Data & Proposed Testing	PHOTODEGRADATION Available Data & Proposed Modeling
68511-50-2 Alkyl Sulfide	0.3% degraded in 28 days	No data located	No data located
67762-55-4 Alkyl Sulfide	No data located	No data located	No data located
72275-86-6	No testing needed Bridging	No testing proposed[1]	Model estimation[2]
122384-85-4 Alkyl Phenate Sulfide	1st Test: 7.8% biodegraded after 28 days 2nd Test: 13.4% biodegraded after 28 days	No data located	No data located

[1] The structures that make up this substance do not contain functional groups that are subject to hydrolytic reactions. Therefore, these materials are expected to be stable in water and no testing is necessary.
[2] AOPWIN, a subroutine in EPIWIN, will be used to model potential indirect photodegradation rates for selected chemical structures that represent these substances.

Table 5. Evaluation of Aquatic Toxicology of Alkenes, C15-C18 alpha, reaction products with sulfurized dodecyl phenol, calcium salt, sulfurized (CAS No. 72275-86-6)

CAS Number	ACUTE TOXICITY TO FISH 96-hr LL_{50} (mg/L)[1]	ACUTE TOXICITY TO INVERTEBRATES 48-hr EL_{50} (mg/L)[1]	TOXICITY TO ALGAE 96-hr EL_{50} (mg/L)[1]
	Available Data & Proposed Testing	**Available Data & Proposed Testing**	**Available Data & Proposed Testing**
68511-50-2 Alkyl sulfide	> 10,000 (WAF^2,S) > 1,000 (WAF^2,F)	> 1,000 (WAF^3, D)	> 100 (WAF^3, P, R) 34 (WAF^3, P, B)
67762-55-4 Alkyl sulfide	No data located	No data located	No data located
72275-86-6	> 10,000 (WAF^2,S)	No testing proposed Bridging	No testing proposed Bridging
122384-85-4 Alkyl phenate sulfide	> 1,000 (WAF^2,F) > 1,000 (WAF^2,T)	> 1,000 (WAF^3, D) >1,000 (WAF^3D) 96 hr EL50 is 2600 mg/L (WAF^2, BS) 96 hr NOEL is 100 mg/L (WAF^2, BS)	> 1,000 (WAF^3, P, B,R) ≥ 1,000 mg/L (algicidal) ≈ 200mg/L (algistatic)

[1]Toxicity endpoints are expressed as median lethal loading rates (LL_{50}) for fish and median effective loading rates (EL_{50}) for *Daphnia* and algae. The EL/LL_{50} is defined as the loading rate that adversely affects 50% of the test organisms exposed to it during a specific time. The greater the EL/LL_{50} the lower the toxicity.
[2]WAF = Water accommodated fraction static renewal test
[3]WAF = Water accommodated fraction static non-renewal test
F = fathead minnow, *Pimephales promelas*
D = freshwater cladoceran, *Daphnia magna*
P = freshwater algae *Pseudokirchneriella subcapitata* formerly called *Selenastrum capricornutum*
T = rainbow trout, *Oncorhynchus mykiss;* formerly called *Salmo gairdneri*
S = sheepshead minnow, *Cyprinodon variegatus*
BS = brown shrimp (*crangon crangon)*
R = growth rate
B = biomass

Table 6. Evaluation of Acute Toxicity of Alkenes, C15-C18 alpha, reaction products with sulfurized dodecyl phenol, calcium salt, sulfurized (CAS No. 72275-86-6)

CAS Number	ACUTE ORAL TOXICITY[1]	ACUTE DERMAL TOXICITY[1]
	Available Data & Proposed Testing	Available Data & Proposed Testing
68511-50-2 Alkyl sulfide	LD_{50} > 5.0 g/kg (rat) LD_{50}>5.0 g/kg (rat)	No data located
67762-55-4 Alkyl sulfide	No data located	LD_{50} > 2.0 g/kg (rabbit)
72275-86-6	LD_{50} > 5.0 g/kg (rat)	LD_{50} > 5.0 g/kg (rabbit)
122384-85-4 Alkyl phenate sulfide	LD_{50} > 5.0 g/kg (rat)	LD_{50} > 2.0 g/kg (rat) LD_{50} > 15.0 g/kg (rabbit)

[1]Toxicity endpoints are expressed as median lethal dose (LD_{50}) for acute oral and dermal toxicity. The LD_{50} is defined as the dose that is lethal to 50% of the test organisms. The greater the LD_{50}, the lower the toxicity.

Table 7. Evaluation of Genetic Toxicity of Alkenes, C15-C18 alpha, reaction products with sulfurized dodecyl phenol, calcium salt, sulfurized (CAS No. 72275-86-6)

CAS Number	GENE MUTATION ASSAY	CHROMOSOMAL ABERRATION ASSAY
	Available Data & Proposed Testing	Available Data & Proposed Testing
68511-50-2 Alkyl Sulfide	Bacterial Reverse Mutation Assay – Not mutagenic	Mouse Micronucleus Assay – Not clastogenic Rat Micronucleus Assay – Not clastogenic
67762-55-4 Alkyl Sulfide	Bacterial Reverse Mutation Assay- Not mutagenic	C12-C16 analog Mouse Micronucleus Assay – Not clastogenic
72275-86-6	Bacterial Reverse Mutation Assay – Not mutagenic	No data located No testing needed Bridging
122384-85-4 Alkyl Phenate Sulfide	Bacterial Reverse Mutation Assay – Not mutagenic	Mouse Micronucleus Assay – Not clastogenic

Table 8. Evaluation of Repeated-dose Mammalian Toxicity of Alkenes, C15-C18 alpha, reaction products with sulfurized dodecyl phenol, calcium salt, sulfurized (CAS No. 72275-86-6)

CAS Number	REPEATED-DOSE TOXICITY	REPRODUCTIVE/DEVELOPMENTAL TOXICITY
	Available Data & Proposed Testing	**Available Data & Proposed Testing**
67124-09-8 Alkyl Sulfide	**28-day repeated dose oral study in rats** NOAEL was not established in this study	One generation reproductive study in rats NOAEL = 50 mg/kg/day
67762-55-4 Alkyl Sulfide	No data located	No data located
72275-86-6	**28-day repeated dose dermal study in rabbits** NOAEL (systemic toxicity) = 100 mg/kg/day	No data located No testing needed Bridging
122384-85-4 Alkyl Phenate Sulfide	**4-week repeated dose oral study in rats** NOAEL = 300 mg/kg/day.	**Oral reproductive/developmental screening study in rats** NOAEL = 1000 mg/kg/day